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Witness assisted eigenspectra solver on a silicon quantum photonic simulator

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Abstract: We demonstrate a new protocol capable of finding ground and excited states of physical Hamiltonians via an eigenstate witness. The experimental test employs a silicon quantum photonic device, embedding arbitrary controlled unitary operations.

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1. Introduction

The characterisation of the spectrum of a given Hamiltonian is a hard task for classical computers, yet it is required to study the properties of a quantum system, and unlock potential applications in a wide range of fields. Quantum simulators offer a promising route to tackle this and other open problems in quantum chemistry. Recently, variational quantum eigensolvers (VQE) have raised increased interest because of their intrinsic error resilience and shallow-depth circuit requirements. These factors make them amenable to near term quantum devices, whilst retaining the peculiar advantages of hybrid quantum-classical methods [1].

Crucially, the analysis of excited states with VQE has for long remained elusive of successful experimental implementations [2,3]. In this contribution we propose and demonstrate a hybrid quantum simulation protocol, representing an eigenspectra solver. Our method requires ansatz-based preparation of target states and the measurement of only the control qubit emerging from a controlled unitary (CU), independently from the size of the Hamiltonian. This measurement provides an estimator of the proximity to an eigenstate: embedded in an objective function, it drives the variational search to improve the initial ansatz. The energy estimate of the approximate eigenstate prepared after the search is refined via Iterative Phase Estimation Algorithm (IPEA). The experimental test employs a SOI quantum photonic chip, with integrated SFWM photon-pair sources, reconfigurable phase shifters and off-chip superconducting single photon detectors (Fig. 1a). Our chip is capable of implementing arbitrary CU without the need for computationally intensive pre-compilations, exploiting the advantages of state-of-art integrated photonic quantum technologies [4].

2. Results

The device schematics is reported in Fig. 1a. The target qubit is composed of two different path-encoded components that go through different unitaries, i.e. $\hat{I}$ and $\hat{U}$, yielding a superposition of circuits as $|0\rangle_C \otimes \hat{I}|\phi\rangle_T + |1\rangle_C \otimes \hat{U}|\phi\rangle_T$. The final part of the target registry provides path information erasing, so that the overall circuit corresponds to a non-compiled CU [5]. The proposed variational search algorithm encodes the dynamics generated by the Hamiltonian in $\hat{U} = e^{-i\hat{H}t}$, thus evolving trial states prepared in the target registry as $|\phi\rangle_T$. Purity of the output control qubit state (P) and an estimator of the energy (E) can be both obtained via state tomography on the control qubit $|\phi\rangle_C$ at each step. In particular, P is provably a sensible measure of the support of $|\phi\rangle_T$ in the eigenbasis of $\hat{H}$, behaving as a *eigenstate witness*: separable two-qubit states emerging from the CU correspond to an eigenstate of $\hat{H}$ being injected as $|\phi\rangle_T$. The phase acquired by $|\phi\rangle_C$ additionally gives information on the corresponding eigenvalue [5]. This allows an objective function $F_{obj} = -\alpha P + \beta E$ to solve for the ground state via a simultaneous energy and purity optimization (not shown here for brevity). Ansätze from classical methods can then provide trial guess states with sufficient overlap with a targeted excited state. Our protocol then maximizes P, updating the choice(s) of trial $|\phi\rangle_T$ at every algorithm step,

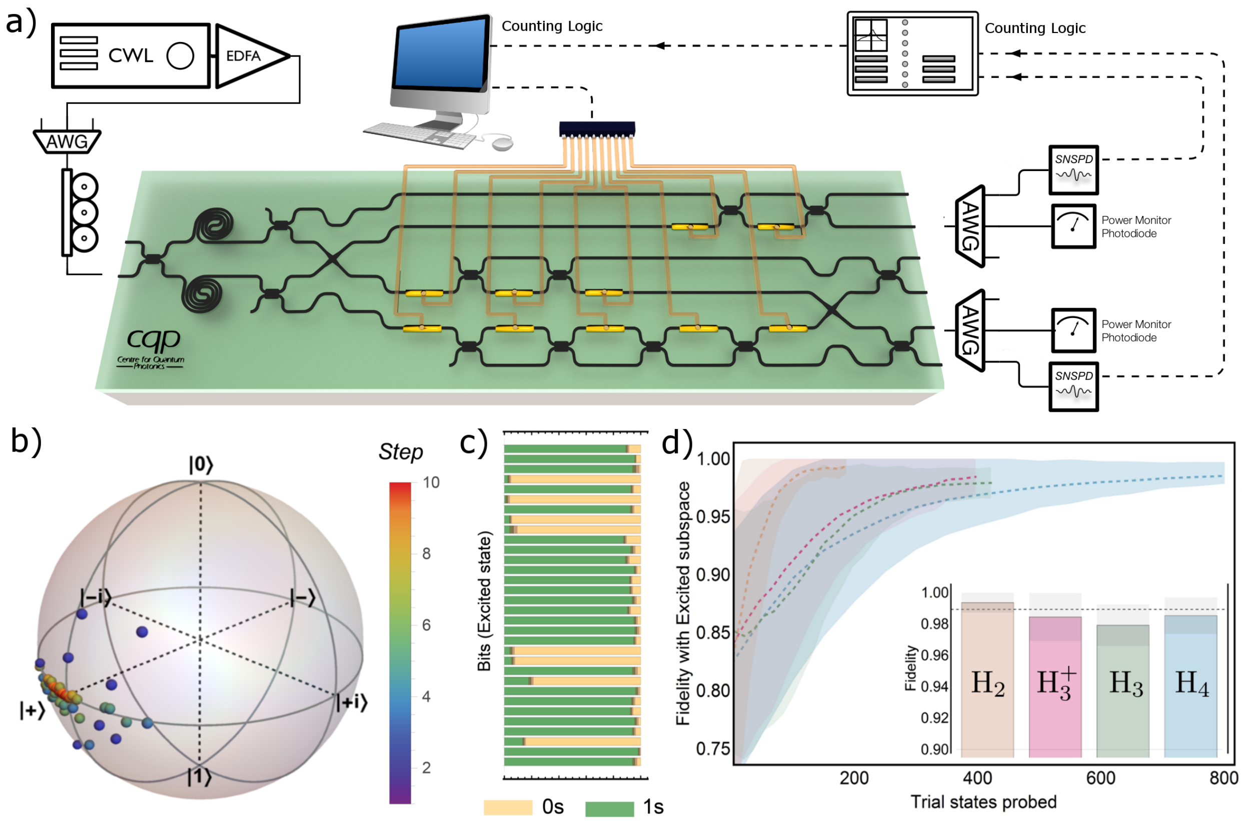

Fig. 1: **a** - Schematic of the 2 qubits device used to implement CU operations, along with basic off-chip components. **b** - Bloch sphere showing the evolution of trial input states $|\phi_T\rangle$, in different colors as per algorithm step, converging to the excited state $|+\rangle$ for the experimentally investigated $\hat{H}$. **c** - Test IPEA run up to 32-bits, for the excited state found. The histogram bars provide experimental normalized coincidence counts, obtained from the projectors of $|\phi_C\rangle$ on the computational basis. **d** - Simulated behaviour of the variational protocol in estimating excited states for test Hamiltonians of different size. Final fidelities achieved are emphasized in the inset with the same color-coding. Shaded areas indicate a 67.5% confidence interval.

variationally refining the initial classical estimate. Fig. 1b shows the variational search for the excited state of a test Hamiltonian, implemented in our photonic device. The swarm of trial states represented on the Bloch sphere is clearly converging to the correct eigenstate $|+\rangle$, up to an average fidelity of 99.8%. In Fig. 1c we demonstrate on our chip how an additional IPEA step is able to provide 32-bits of accuracy in the energy estimate for the found eigenstate. The potential of our method for Hamiltonians beyond the capabilities of the photonic chip has been explored in numerical simulations for Hydrogen molecules up to H_8 (Fig 1d), yielding average fidelities higher than 99%.

In conclusion, our method combines the advantages of variational protocols and quantum phase estimation, introducing a concept with no classical equivalent, the eigenstate witness, that allows to extend the capabilities of variational eigensolvers to target excited states experimentally for the first time.

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